wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 10:07 pm GMT

PDB ID	:	1O7D
Title	:	The structure of the bovine lysosomal a-mannosidase suggests a novel mechanism for low pH activation
Authors	:	Heikinheimo, P.; Helland, R.; Leiros, H.S.; Leiros, I.; Karlsen, S.; Evjen, G.; Ravelli, R.; Schoehn, G.; Ruigrok, R.; Tollersrud, O.-K.; Mcsweeney, S.; Hough, E.
Deposited on	:	2002-10-30
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

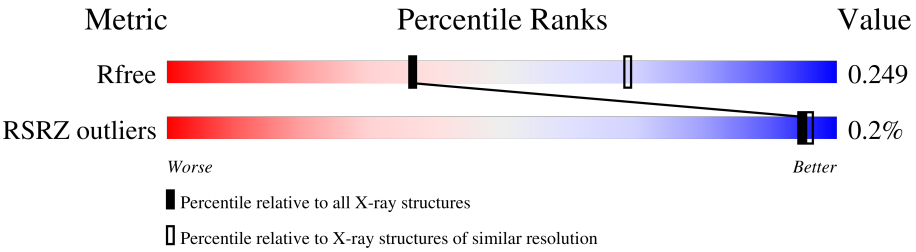
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	F	1	X	-	-	-
7	NAG	G	2	X	-	-	-

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 7385 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lysosomal alpha-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	1
			2365	1520	408	426	11			

- Molecule 2 is a protein called Lysosomal alpha-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	76	Total	C	N	O	S	0	0	1
			622	409	101	109	3			

- Molecule 3 is a protein called Lysosomal alpha-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	151	Total	C	N	O	S	0	0	1
			1136	722	194	214	6			

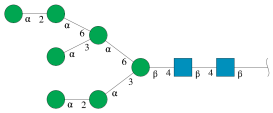
- Molecule 4 is a protein called Lysosomal alpha-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	270	Total	C	N	O	S	0	0	1
			2150	1356	397	392	5			

- Molecule 5 is a protein called Lysosomal alpha-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	109	Total	C	N	O	S	0	0	1
			851	543	148	159	1			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

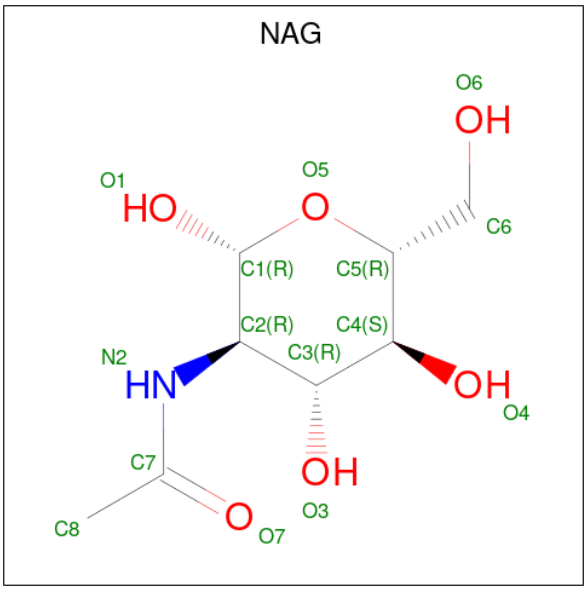


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	F	9	Total C N O 105 58 2 45	0	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

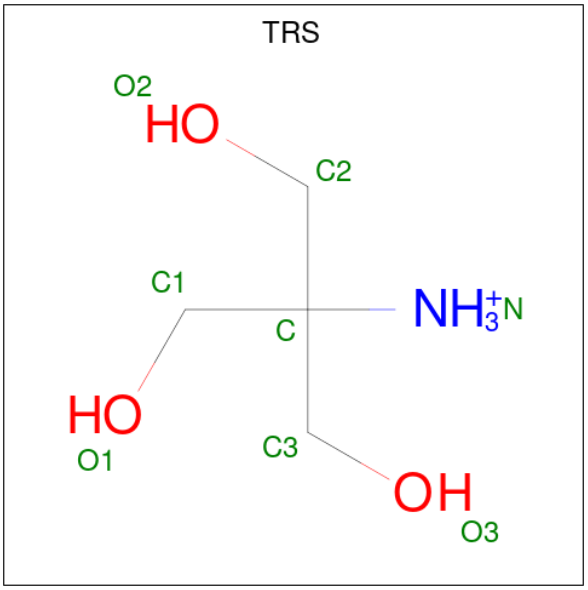
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	G	2	Total C N O 28 16 2 10	0	0	0
7	H	2	Total C N O 28 16 2 10	0	0	0
7	I	2	Total C N O 28 16 2 10	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	A	1	14	8	1	5	0	0

- Molecule 9 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).

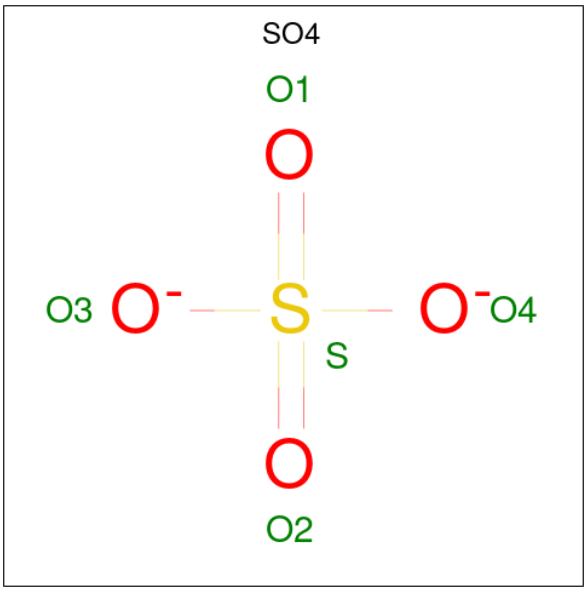


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	A	1	8	4	1	3	0	0

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
10	A	1	1	1	0	0

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total O S 5 4 1	0	0
11	E	1	Total O S 5 4 1	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	14	Total O 14 14	0	0
12	B	2	Total O 2 2	0	0
12	C	3	Total O 3 3	0	0
12	D	14	Total O 14 14	0	0
12	E	6	Total O 6 6	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	117.88Å 117.88Å 582.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.62 – 2.51	Depositor EDS
% Data completeness (in resolution range)	89.4 (30.00-2.70) 86.0 (29.62-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.257 , 0.289 0.252 , 0.249	Depositor DCC
R_{free} test set	3584 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	45.3	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7385	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates

15 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	F	1	6,3	14,14,15	0.59	0	17,19,21	1.24	1 (5%)
6	NAG	F	2	6	14,14,15	0.57	0	17,19,21	0.86	1 (5%)
6	BMA	F	3	6	11,11,12	0.43	0	15,15,17	0.61	0
6	MAN	F	4	6	11,11,12	0.47	0	15,15,17	0.89	1 (6%)
6	MAN	F	5	6	11,11,12	0.53	0	15,15,17	0.72	0
6	MAN	F	6	6	11,11,12	0.41	0	15,15,17	0.72	1 (6%)
6	MAN	F	7	6	11,11,12	0.57	0	15,15,17	0.51	0
6	MAN	F	8	6	11,11,12	0.83	1 (9%)	15,15,17	0.91	0
6	MAN	F	9	6	11,11,12	1.69	2 (18%)	15,15,17	3.02	4 (26%)
7	NAG	G	1	4,7	14,14,15	0.76	0	17,19,21	0.97	1 (5%)
7	NAG	G	2	7	14,14,15	0.82	0	17,19,21	1.15	2 (11%)
7	NAG	H	1	4,7	14,14,15	0.54	0	17,19,21	0.94	1 (5%)
7	NAG	H	2	7	14,14,15	0.59	0	17,19,21	0.74	0
7	NAG	I	1	4,7	14,14,15	0.75	0	17,19,21	1.05	1 (5%)
7	NAG	I	2	7	14,14,15	0.62	0	17,19,21	0.87	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	F	1	6,3	1/1/5/7	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	2/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	MAN	F	4	6	-	0/2/19/22	0/1/1/1
6	MAN	F	5	6	-	1/2/19/22	0/1/1/1
6	MAN	F	6	6	-	0/2/19/22	0/1/1/1
6	MAN	F	7	6	-	2/2/19/22	0/1/1/1
6	MAN	F	8	6	-	2/2/19/22	0/1/1/1
6	MAN	F	9	6	-	1/2/19/22	0/1/1/1
7	NAG	G	1	4,7	-	2/6/23/26	0/1/1/1
7	NAG	G	2	7	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	H	1	4,7	-	4/6/23/26	0/1/1/1
7	NAG	H	2	7	-	5/6/23/26	0/1/1/1
7	NAG	I	1	4,7	-	6/6/23/26	0/1/1/1
7	NAG	I	2	7	-	4/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	9	MAN	C1-C2	-3.31	1.44	1.52
6	F	9	MAN	O5-C1	3.11	1.48	1.43
6	F	8	MAN	C2-C3	2.25	1.55	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	9	MAN	C1-C2-C3	7.10	118.39	109.67
6	F	9	MAN	C6-C5-C4	6.58	128.42	113.00
6	F	9	MAN	O3-C3-C2	-3.90	102.52	109.99
6	F	9	MAN	C1-O5-C5	3.78	117.31	112.19
6	F	1	NAG	O5-C1-C2	3.39	116.65	111.29

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	F	1	NAG	C1
7	G	2	NAG	C1

5 of 35 torsion outliers are listed below:

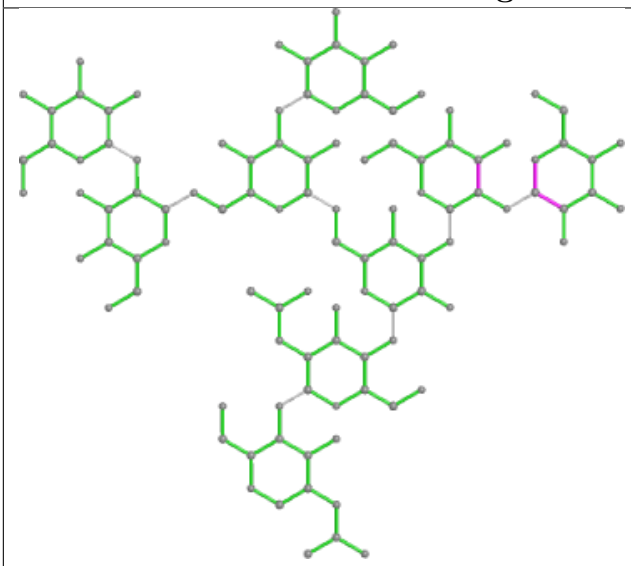
Mol	Chain	Res	Type	Atoms
6	F	1	NAG	C8-C7-N2-C2
6	F	1	NAG	O7-C7-N2-C2
7	G	2	NAG	C8-C7-N2-C2
7	G	2	NAG	O7-C7-N2-C2
7	H	1	NAG	C8-C7-N2-C2

There are no ring outliers.

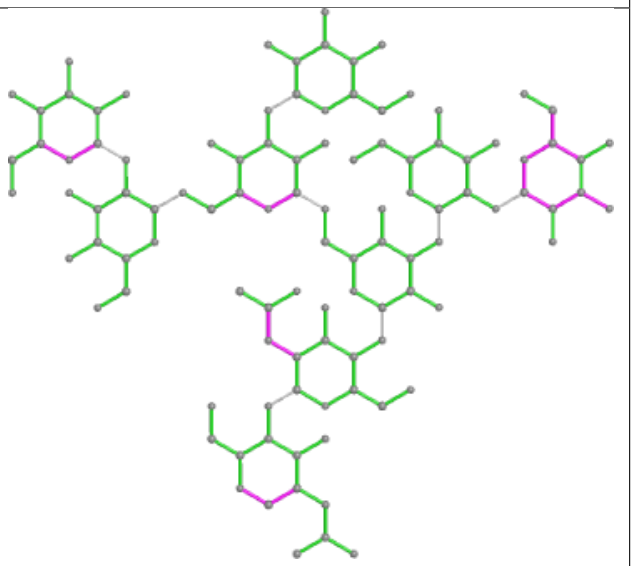
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

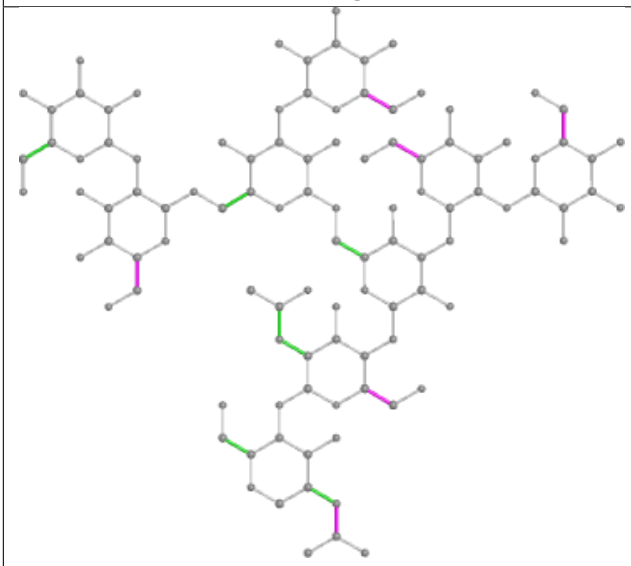
Oligosaccharide Chain F



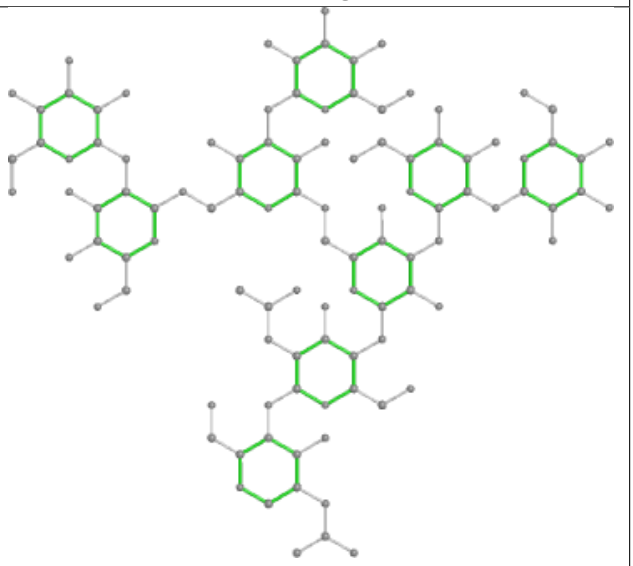
Bond lengths



Bond angles

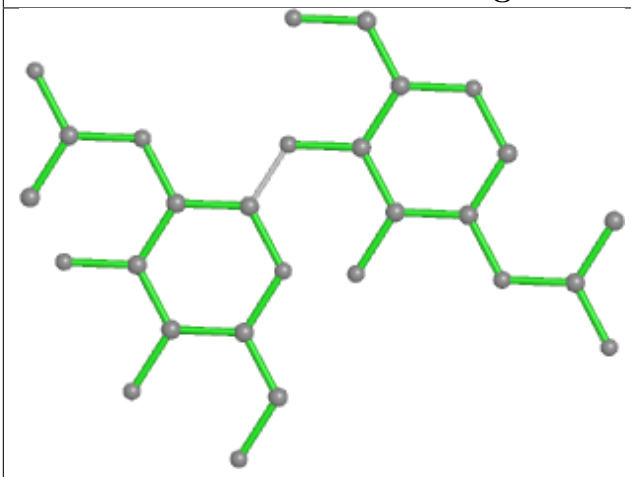


Torsions

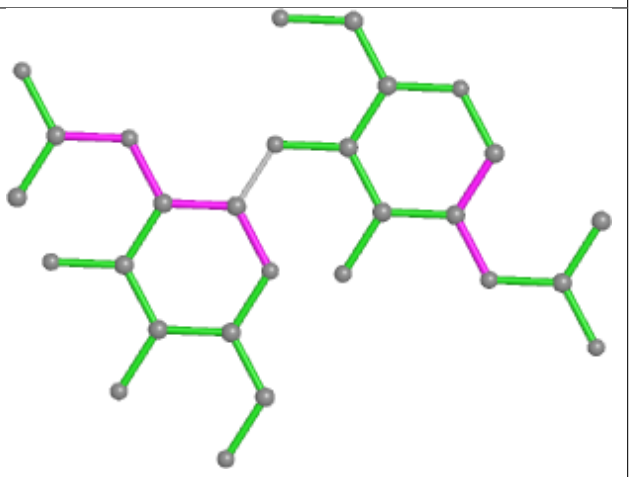


Rings

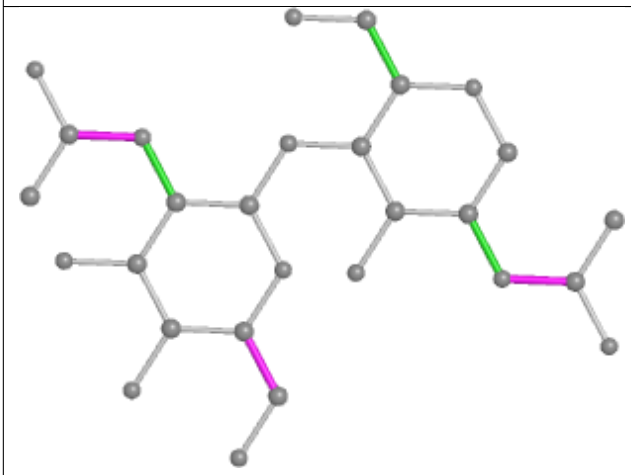
Oligosaccharide Chain G



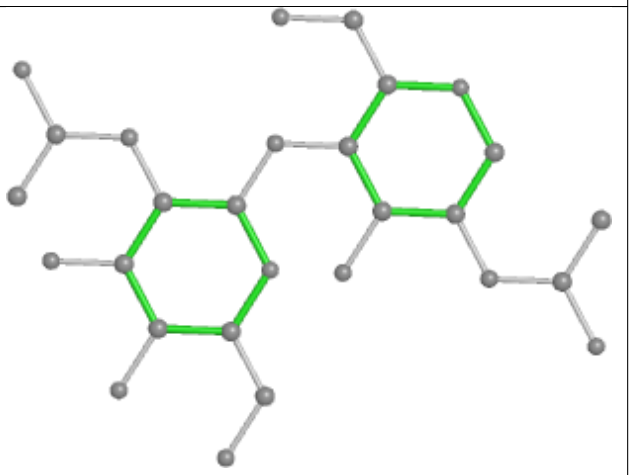
Bond lengths



Bond angles

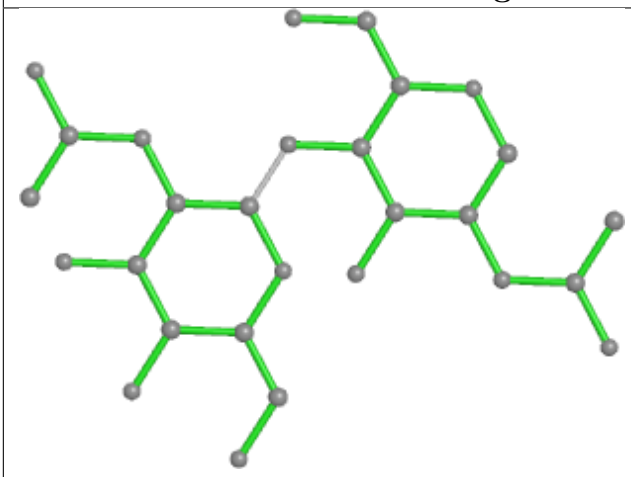


Torsions

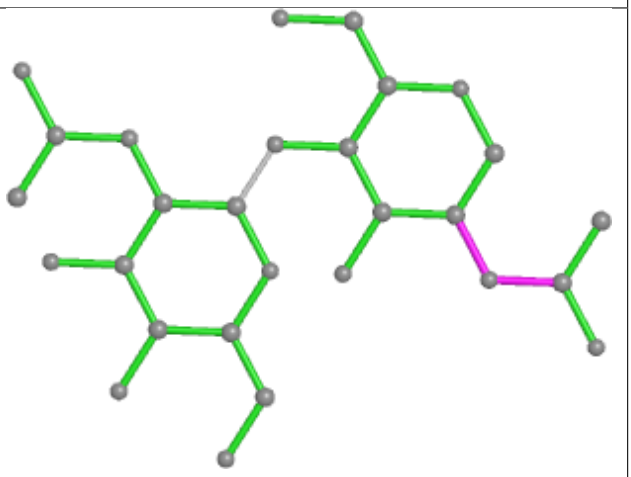


Rings

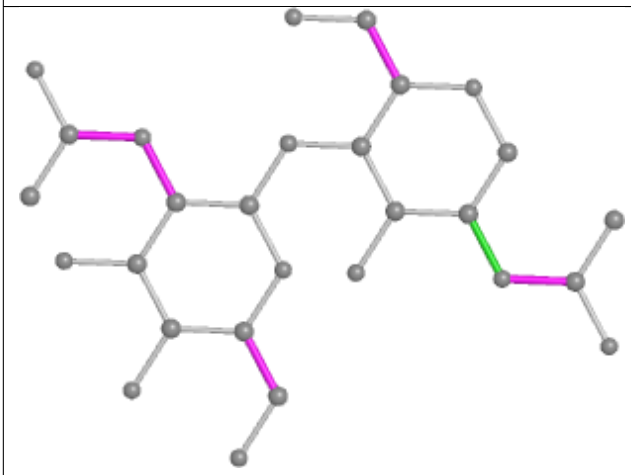
Oligosaccharide Chain H



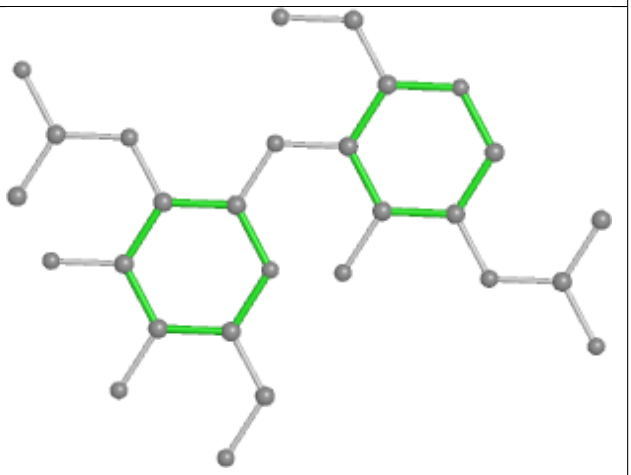
Bond lengths



Bond angles

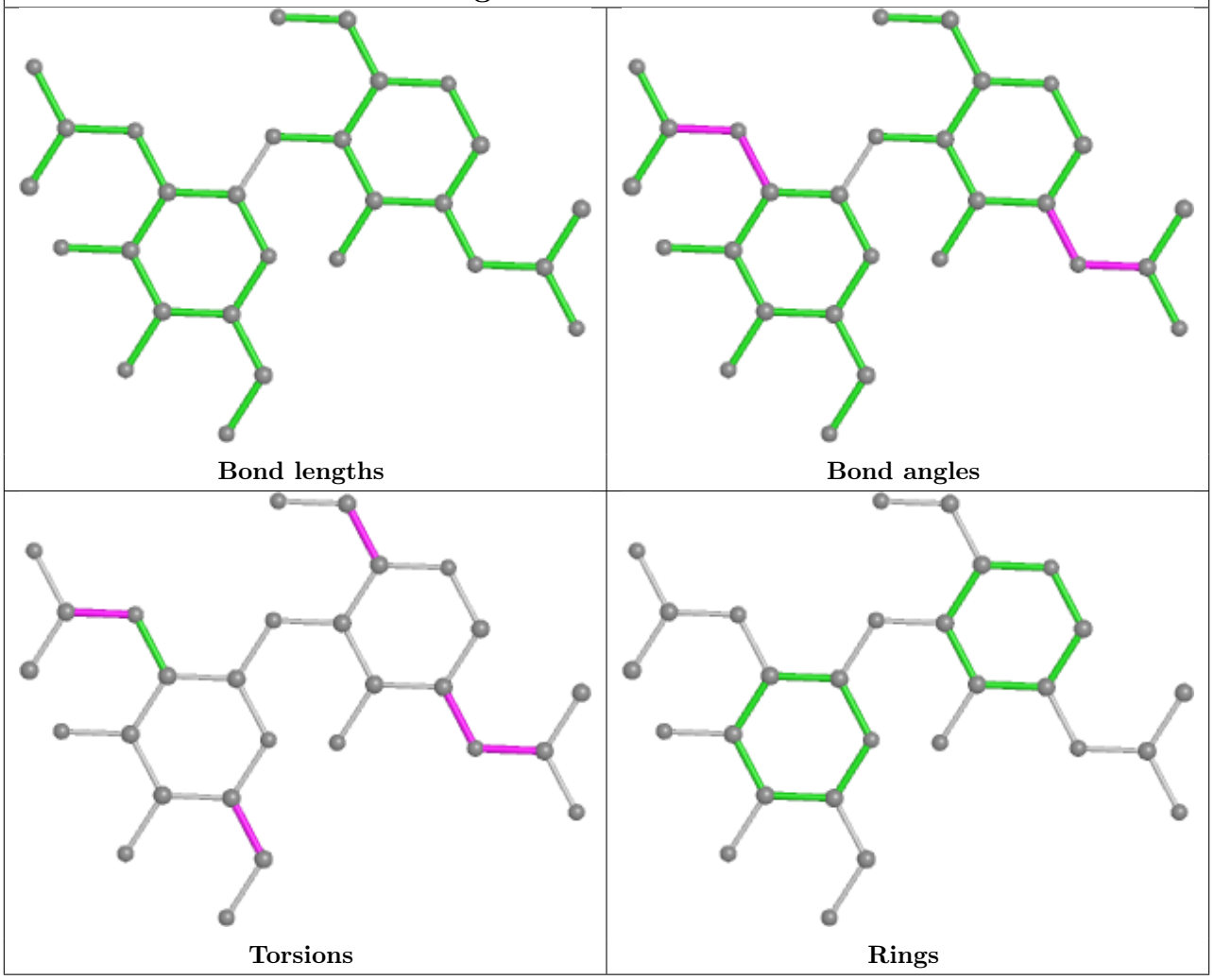


Torsions



Rings

Oligosaccharide Chain I



4.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	SO4	A	3001	-	4,4,4	0.53	0	6,6,6	0.23	0
8	NAG	A	1	1	14,14,15	0.70	0	17,19,21	0.79	0
11	SO4	E	3002	-	4,4,4	0.64	0	6,6,6	0.15	0
9	TRS	A	2	10	7,7,7	1.50	2 (28%)	9,9,9	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1	1	-	6/6/23/26	0/1/1/1
9	TRS	A	2	10	-	0/9/9/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2	TRS	C2-C	2.17	1.60	1.53
9	A	2	TRS	C-N	-2.07	1.42	1.49

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1	NAG	C3-C2-N2-C7
8	A	1	NAG	C8-C7-N2-C2
8	A	1	NAG	O7-C7-N2-C2
8	A	1	NAG	C4-C5-C6-O6
8	A	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	292/298 (97%)	-0.59	0 100 100	22, 36, 54, 76	0
2	B	76/84 (90%)	-0.51	1 (1%) 77 78	18, 35, 70, 87	0
3	C	151/159 (94%)	-0.67	0 100 100	22, 36, 56, 95	0
4	D	270/282 (95%)	-0.54	1 (0%) 92 93	21, 38, 58, 94	0
5	E	109/126 (86%)	-0.66	0 100 100	16, 38, 59, 92	0
All	All	898/949 (94%)	-0.59	2 (0%) 95 96	16, 37, 58, 95	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	422	ALA	3.6
4	D	875	GLY	2.3

5.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MAN	F	9	11/12	0.83	0.18	72,72,72,72	0
7	NAG	G	2	14/15	0.85	0.32	79,79,79,79	0
6	MAN	F	7	11/12	0.89	0.19	57,57,57,57	0

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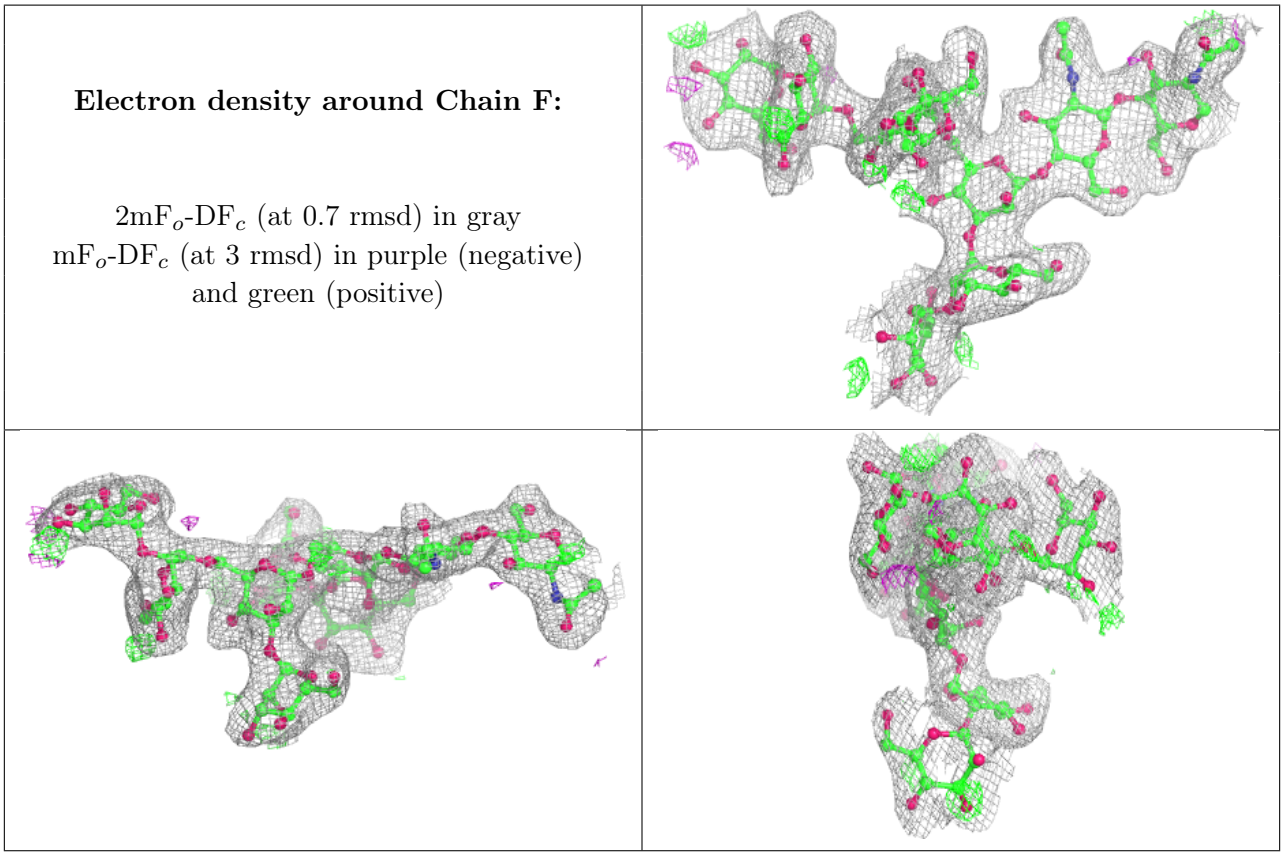
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	H	2	14/15	0.90	0.22	67,67,67,67	0
7	NAG	I	2	14/15	0.91	0.28	75,75,75,75	0
6	MAN	F	5	11/12	0.92	0.14	32,32,32,32	0
7	NAG	H	1	14/15	0.92	0.10	46,46,46,46	0
7	NAG	G	1	14/15	0.93	0.18	50,50,50,50	0
7	NAG	I	1	14/15	0.94	0.20	44,44,44,44	0
6	MAN	F	4	11/12	0.94	0.11	33,33,33,33	0
6	MAN	F	8	11/12	0.95	0.14	44,44,44,44	0
6	NAG	F	1	14/15	0.95	0.12	31,31,31,31	0
6	MAN	F	6	11/12	0.96	0.10	27,27,27,27	0
6	NAG	F	2	14/15	0.96	0.10	25,25,25,25	0
6	BMA	F	3	11/12	0.97	0.10	33,33,33,33	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

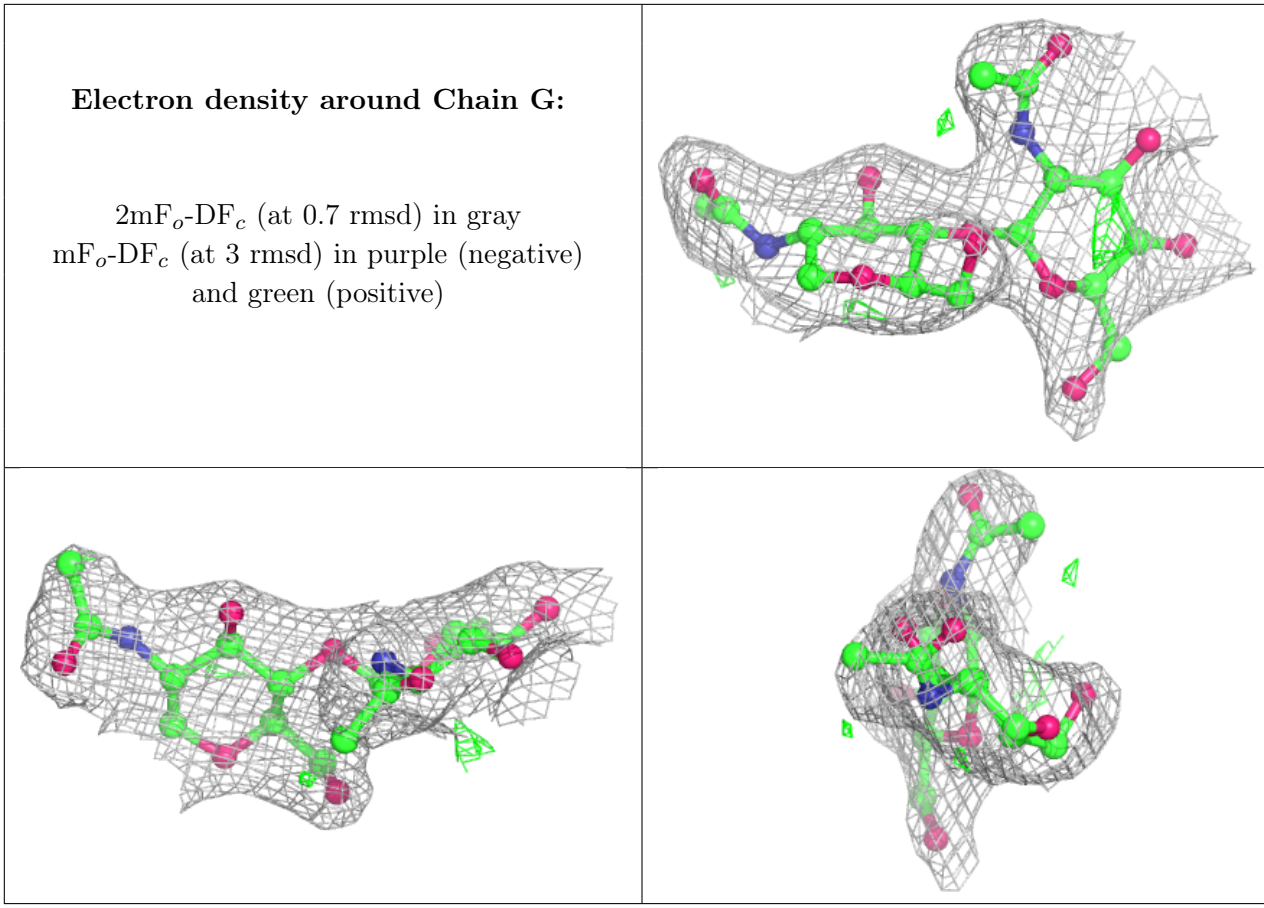
Electron density around Chain F:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



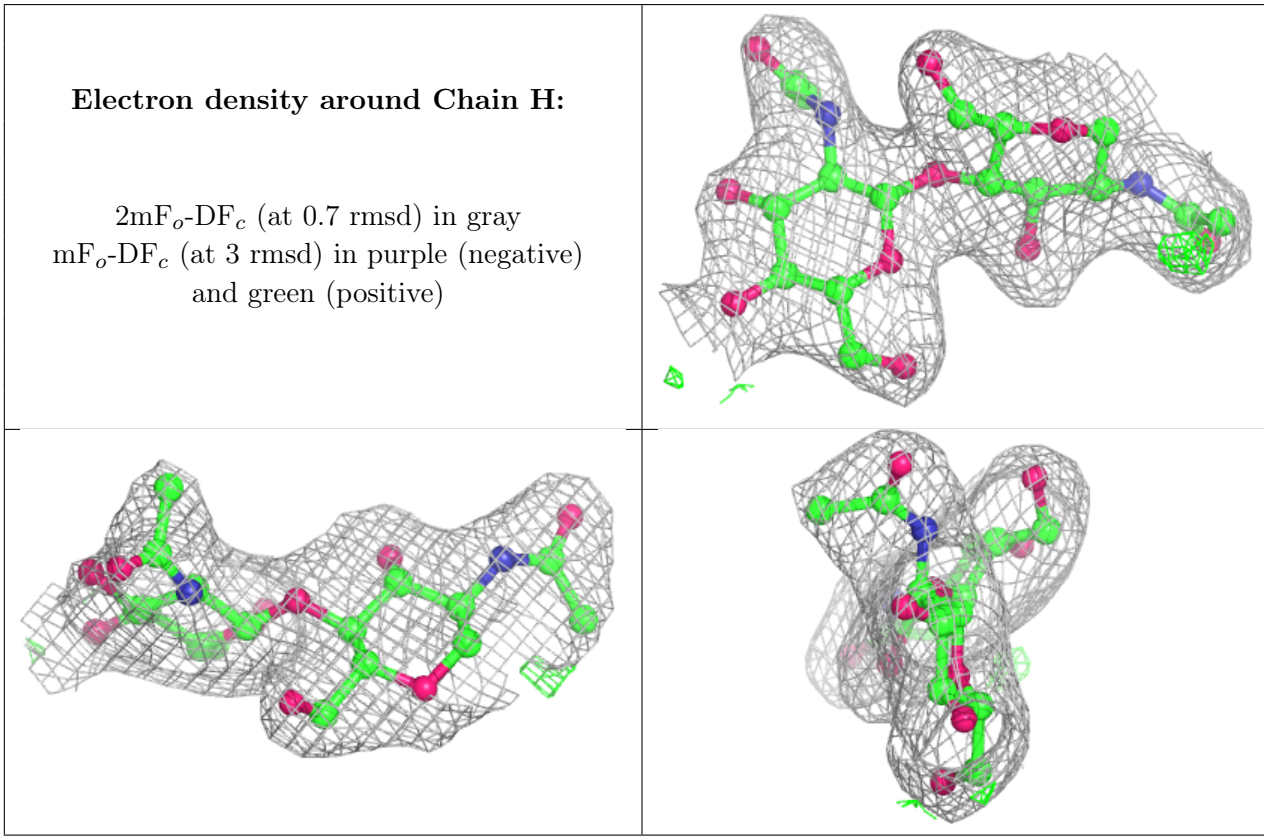
Electron density around Chain G:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



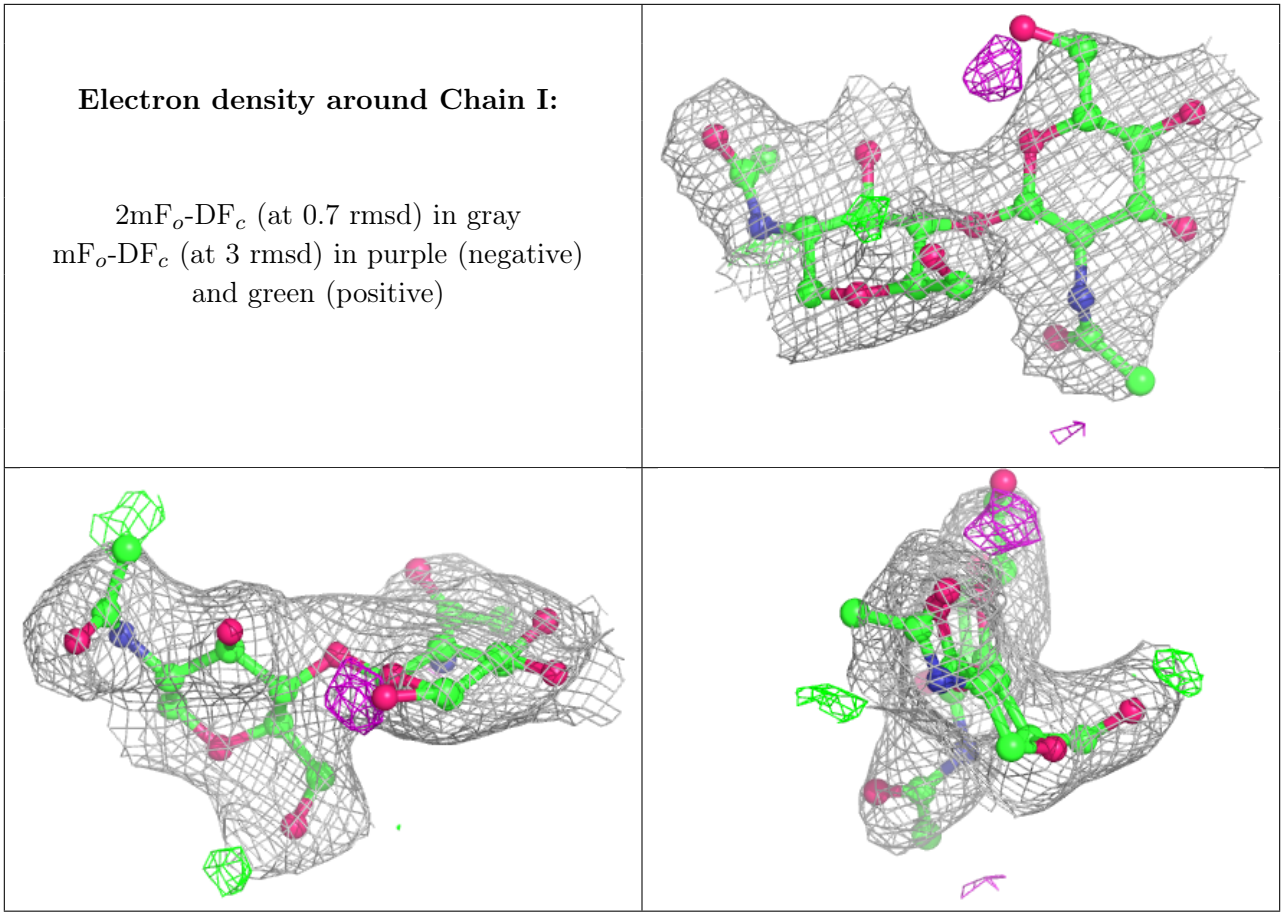
Electron density around Chain H:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain I:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



5.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	A	1	14/15	0.84	0.32	57,57,57,57	0
9	TRS	A	2	8/8	0.87	0.23	35,35,35,35	0
11	SO4	A	3001	5/5	0.96	0.20	36,36,36,36	0
11	SO4	E	3002	5/5	0.98	0.14	36,36,36,36	0
10	ZN	A	3	1/1	0.99	0.11	35,35,35,35	0

5.5 Other polymers

There are no such residues in this entry.